Hello Bio, Inc. 304 Wall St., Princeton, NJ 08540 USA

T. 609-683-7500 F. 609-228-4994

customercare-usa@hellobio.com



# **DATASHEET**

Cmpd101

### **Product overview**

 Name
 Cmpd101

 Cat No
 HB2840

Alternative names Compound 101; Takeda compound 101

**Biological action** Inhibitor Purity >98%

Customer comments We would recommend Cmpd 101 from Hello Bio – it performs exactly as expected in assays looking

at MOPr desensitisation, phosphorylation and internalisation. Dr Chris Bailey, University of Bath,

UK and author on Mol Pharmacol paper, PubMed ID 26013542

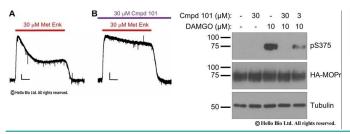
Your Cmpd101 - worked great! Dr Steven Gee, Pfizer Neuroscience, USA

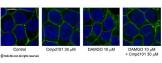
Your Cmpd101 behaved as expected. Verified customer, Monash University

Novel, potent and selective GRK2/GRK3 inhibitor

### **Images**

Description







### **Biological Data**

**Biological description** 

Cmpd101 (Compound 101) is a novel, potent and selective G-protein coupled receptor kinase 2 and 3 (GRK2/GRK3) inhibitor ( $IC_{50}$  values are 35 and 32 nM at GRK2 and GRK3 respectively).

Shows no activity at GRK5 at concentrations up to 125  $\mu$ M and shows little activity at a broad range of other kinases.

Membrane permeable.

Cmpd101 can be used to study roles of GRK2/3 in GPCR desensitization and other functions.

Shown to potentiate phosphatidylinositol 4,5-bisphosphate (PIP2) depletion and slow agonist-induced desensitization of protease-activated receptor 2 (PAR2).

## **Solubility & Handling**

Storage instructions -20°C

Prepare and use solutions on the same day if possible. Store solutions at -20 °C for up to one month if Storage of solutions

storage is required. Equilibrate to RT and ensure the solution is precipitate free before use.

Hydroscopic solid, contact with air may cause material to become sticky. Product performance should

not be affected but we recommend storing the material in a sealed jar.

**Shipping Conditions** 

**Important** 

Handling

Stable for ambient temperature shipping. Follow storage instructions on receipt.

This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not

for human or veterinary use.

### **Chemical Data**

Chemical name 3-[(4-methyl-5-pyridin-4-yl-1,2,4-triazol-3-yl)methylamino]-N-[[2-(trifluoromethyl)phenyl]methyl]benzam

ide hydrochloride

Molecular Weight 502.92

**Chemical structure** 

Molecular Formula C<sub>24</sub>H<sub>21</sub>N<sub>6</sub>OF<sub>3</sub>.HCl **CAS Number** 865608-11-3 **PubChem identifier** 11677079

**SMILES** CN1C(=NN=C1C2=CC=NC=C2)CNC3=CC=CC(=C3)C(=O)NCC4=CC=CC=C4C(F)(F)F

Source Synthetic

InChi InChI=1S/C24H21F3N6O/c1-33-21(31-32-22(33)16-9-11-28-12-10-16)15-29-19-7-4-6-17(13-19)23(

34)30-14-18-5-2-3-8-20(18)24(25,26)27/h2-13,29H,14-15H2,1H3,(H,30,34)

WFOVEDJTASPCIR-UHFFFAOYSA-N InChiKey

Yellow solid **Appearance** 

#### References

Molecular mechanism of selectivity among G protein-coupled receptor kinase 2 inhibitors.

Thal et al (2011) Mol Pharmacol 80

**PubMedID** 21596927

Role of G Protein-Coupled Receptor Kinases 2 and 3 in μ-Opioid Receptor Desensitization and Internalization.

Lowe et al (2015) Mol Pharmacol 88(2) **PubMedID** 26013542

Contributions of protein kinases and β-arrestin to termination of protease-activated receptor 2 signaling.

Jung et al (2016) J Gen Physiol 147(3)

**PubMedID** 26927499

Distinct cortical and striatal actions of a β-arrestin-biased D2 receptor ligand reveal unique antipsychotic-like properties.

Urs et al (2016) Proc Natl Acad Sci U S A 113(50) **PubMedID** 27911814

Agonist-selective recruitment of engineered protein probes and of GRK2 by opioid receptors in living cells

Stoeber et al (2019) bioRxiv https://doi.org/10.1101/866780